

Supplementary Data

Guidelines for Deposition of Supplementary Data†

Also see: www.rsc.org/authorguidelines

CONTENTS

1.0 Electronic Supplementary Information

- 1.1 Introduction
- 1.2 Text and graphics
- 1.3 Significant structures
- 1.4 Crystallographic Information Files (CIFs)
- 1.5 3D files, spectral data files and movies

2.0 Crystallographic data

3.0 Externally deposited data

1.0 Electronic Supplementary Information

1.1 Introduction

The RSC's Electronic Supplementary Information (ESI) service is a free facility that enables authors to enhance and increase the impact of their articles. Authors are encouraged to make the most of the benefits of publishing supplementary information in electronic form. Such data can take full advantage of the electronic medium, allowing use of full colour diagrams, 3D molecular models and even movies. Authors can also improve the readability of their articles by placing appropriate material, such as repetitive experimental details and bulky data, with the ESI service. All information in the ESI service is also fully archived.

Authors wishing to submit electronic supplementary information for an article should, where possible, supply data in one of the formats described in the 'Acceptable Formats' section of the RSC web site.† Other formats may be supplied, and every effort will be made to use these where possible. It is intended that the ESI system should make full use of developing file types to allow authors to present their data in the most useful and interesting ways possible. If you are providing an unusual file type, please provide the Editorial Office with details of any additional software that would be required to view the files. Such software should be available freely, preferably via the web.

When preparing their ESI data files, authors should keep in mind the following points:

- ESI files are usually published 'as is'—Editorial staff won't normally edit the data for style or content
- Data is only useful if readers can access it—use common, widely known file formats

- Large files may prove difficult for users to download and access

1.2 Text and graphics

The preferred format for ESI comprising text and graphics is Adobe's Portable Document Format (PDF), as this format can be accessed easily and reliably on most computing platforms using the freely available Adobe Acrobat Reader. For information on creating PDF files, see the 'Acceptable Formats' section of the RSC web site.† Text files created using one of the other 'Acceptable Formats' can be submitted, however Editorial staff may convert them to PDF files before publication. Static 2D graphic files are best submitted as either PDF files (see above) or as GIF or JPEG files (maximum size 640 by 480 pixels). If other formats are submitted they will usually be converted to PDF files prior to publication.

1.3 Significant structures

Significant chemical structures can be made freely available for download as part of the ESI service. These should be supplied as either ChemDraw or ISISDraw files using the appropriate template.†

1.4 Crystallographic Information Files (CIFs)

CIFs should be created in accordance with the instructions given in the 'Acceptable Formats' section of the RSC web site.† Authors are also encouraged to use their CIFs to produce 3D molecular files.

1.5 3D files, spectral data files and movies

These file types exploit electronic publishing systems to the full, and authors are strongly encouraged to make use of them to support and enhance their articles. Files should be created in accordance with the instructions given in the 'Acceptable Formats' section of the RSC web site.†

In addition, *Molecular BioSystems* now offers a new service that enables the 3D visualisation of complex molecules. This is made possible by using the PDB identification code to generate an image using FirstGlance in Jmol.‡ To take advantage of this service, please provide the PDB identification code at submission.

2.0 Crystallographic data

Supplementary crystallographic data will be deposited by the RSC with the Cambridge Crystallographic Data Centre (CCDC) as part of the assessment process. Each structure will be assigned a

† For more detailed information on this topic, as well as links to useful websites and software resources, see: <http://www.rsc.org/authorguidelines>.

‡ See <http://firstglance.jmol.org> for details.

separate CCDC number that will be quoted in the subsequent crystallographic report. Data will be held in the CCDC's confidential archive until publication of the article, when data for organic and metallo-organic compounds will be entered into the Cambridge Structural Database, and data for inorganic compounds will be forwarded to Fachinformationszentrum Karlsruhe for inclusion in the Inorganic Crystal Structure Database. Post-publication requests for individual data sets (organic or inorganic) should be directed to the CCDC.

If the article is not published by the RSC, supplementary crystallographic data will remain in the CCDC's confidential archive. If the crystal structure(s) are subsequently published elsewhere, the CCDC Deposition Number(s) provided in the RSC crystallographic report should be quoted in that publication, and the CCDC advised of the new journal and the appropriate reference. Data will then enter the appropriate database as described above.

3.0 Externally deposited data

Novel macromolecular structures and newly reported nucleic acid or protein sequences and microarray data must be deposited with

§ Worldwide Protein Data Bank: <http://www wwpdb.org>; Nucleic Acids Database: <http://ndbserver.rutgers.edu/>; National Center for Biotechnology Information (GenBank): <http://www.ncbi.nlm.nih.gov/>; DNA Data Bank of Japan: <http://www.ddbj.nig.ac.jp/>; SWISS-PROT: <http://www.ebi.ac.uk/swissprot/>; Protein Information Resource (Protein Sequence Database): <http://pir.georgetown.edu/>; Gene Expression Omnibus (GEO): <http://www.ncbi.nlm.nih.gov/geo/>; ArrayExpress: <http://www.ebi.ac.uk/arrayexpress/>.

the appropriate database. § Articles will not be published until the relevant accession number has been provided. These codes should be quoted both in the experimental section of the manuscript and in the abstract (or article header information) so that abstracting services will access them. Microarray data should be MAIME compliant. ¶

For X-ray structures, atomic coordinates and structure factor data are required. For NMR structures, data should include all resonance assignments and restraints used in structure determination (NOEs, spin-spin coupling constants, amide exchange rates, *etc.*) as well as atomic coordinates derived for both an individual/average structure and an acceptable family of structures.

Sufficient information must be supplied to satisfy referees of the validity of the conclusions drawn. For X-ray structures, PDB header information (*i.e.* Rmerge, completeness, multiplicity and I/sigmaI (both overall and in the outer resolution shell) for data, and Rcryst, Rfree and the bond and angle deviations for coordinates), a Ramachandran plot and preferably real space R-factor must be supplied. For NMR structures equivalent data (number of restraints (NOEs and J-couplings), RMS restraint deviation *etc.*) plus resonance assignments in the case of NMR structures must be supplied. All the above data should be included in as summary data tables in the manuscript, or as ESI.

Reference may also be made to data deposited with PubChem. || Suitable links should be provided as footnotes to the text of the article.

¶ See <http://www.mged.org/workgroups/MIAME/miame.html> for details.

|| See <http://pubchem.ncbi.nlm.nih.gov/> for details.